Chapter 6
Mathematical Modelling

Abstract Modelling of biomass combustion using Computational Fluid Dynamics (CFD) is covered in the chapter. The Reynolds-Averaged Navier-Stokes equations are outlined as well as turbulence-chemistry interactions. Modelling pulverised biomass particle combustion is outlined including the sub-models. These are particle motion, heat transfer, devolatilisation and char combustion. Modelling pulverised fuel co-firing in power stations is next considered using the methods outlined previously. Modelling fixed and fluidised bed combustion is then described. The application of these methods to model the emission of nitrogen and sulphur oxide emissions and aerosol pollutants is outlined.

Keywords Combustion modelling techniques · Pollutant formation · Metal aerosols

6.1 Modelling Biomass Combustion Using Computational Fluid Dynamics

Computational Fluid Dynamics (CFD) modelling has been developed as an important tool for the design, optimization and prediction of pollutants from large pulverised coal combustion plants and these techniques have been extended to co-firing coal and biomass (Williams et al. 2001). Some work has been devoted to modelling firing 100 % pulverised biomass systems but little is published because they are not widely used at present. CFD studies of emissions from fixed and fluidised bed combustion of biomass have been published over the last decade as well as some work on incineration where the fuel is assumed to have a biomass-like composition. Over the past decade, combustion modelling using CFD has been transformed from qualitative modelling to quantitative predictions in many engineering applications. A number of commercial CFD software packages are now available that are capable of providing reasonable simulations for solid fuel combustion, with user defined specific sub-models which are employed in the coal/biomass combustion modelling applications. Modelling techniques have been developed for various degrees of complexity. Currently, three-dimensional simulations for full-scale furnaces with millions of computational cells are achievable.

© The Author(s) 2014

J.M. Jones et al., *Pollutants Generated by the Combustion of Solid Biomass Fuels*,
SpringerBriefs in Applied Sciences and Technology,
DOI 10.1007/978-1-4471-6437-1_6

CFD combustion modelling is based on the solution of a set of fundamental conservation equations that govern the general reacting flows incorporating fuel specific processes. The bases of these are set out in a number of text books as well as the solution techniques available (For example: Andderson et al. 2012; Chung 2002; Wendt 2009). Solid fuel combustion involves the follow five main tasks:

1. Gas phase flow and volatile combustion modeling, including pollutant predictions,
2. Particle fluid dynamics modelling and inter-phase heat/mass transfer,
3. Devolatilisation modelling,
4. Heterogeneous char combustion modelling, and
5. Reactions of inorganic species including condensation and deposition.

CFD modelling was initially used for geometrically simple gaseous and spray flames with single step combustion chemistry. These spray models were developed into models of pulverised coal combustion because of the similarity of the combustion process as well as the handling of the particulate systems. Application to fixed bed combustion was only developed recently and initially took the approach that a simple fixed bed model produced combustible gases above the bed that then reacted in the gas phase. These models have become more sophisticated including the dynamic motion of the bed. These models have been extended to fluidised bed combustion but little work has been undertaken on the combustion of biomass.

We have a good knowledge about modelling pulverised coal combustion and it is generally accepted that many aspects of the combustion of pulverised biomass are similar to that of coal. Thus these models were adapted and/or with some modifications to the biomass combustion. Here two fundamental modeling approaches exist. These are the Eularian-Eularian and the Eularian-Largragian approaches. In the Eularian method, the discrete solid phase is also considered as a continuum. Therefore the Eulerian conservation equations are solved for both the gas and the suspended particulate phases and the model can include all the stages of a particle combustion process, particle drag and turbulent dispersions, etc. The distinctive benefit of the Eulerian-Eulerian approach is its computational efficiency which is the result from the elimination of the particle tracking and iterations and corrections between dispersed particles and the continuum phase. The Eularian-Lagrangian method, which is the predominant simulation procedure for pulverised solid fuel combustions, solves the motion of combusting particles by tracking them separately in a Lagrangian reference frame, whilst the gas phase is solved in the Eulerian domain. Most solid fuel combustion submodels are designed for this approach.

In the Eularian-Lagrangian approach, the fluid flow and volatile combustion are modelled by solving the time-averaged equations of global mass, momentum, energy, and species mass fractions within an Eulerian reference frame. Turbulence models and turbulence-chemistry interaction schemes are incorporated to simulate the effect of turbulence on the reacting flow. These equations may be solved by using general CFD numerical solution technique such as the control volume method or the finite element method. Pulverized fuel particles are typically treated as dilute and dispersed particulate flows and they are modelled in a Lagrangian reference frame where the particle motion and reaction are tracked step-by-step by time throughout the combustion system. The assumption behind this approach is that the distance between any two fuel particles is large that any chance of particle interactions is small and therefore may be ignored. With this assumption, the movement and the heterogeneous reaction of each combusting particle stream is tracked individually by a set of Lagrangian formulations. The coupling of the gaseous and the solid phases is established through the source/sink terms of mass, momentum and energy in the Eulerian gas-phase conservation equations, and the overall solution involves a multi-loop iterative procedure.

A general solution strategy for modelling the co-firing of biomass and coal within the Eularian-Lagrangian framework is illustrated as in Fig. 6.1. The overall iterative solution process begins by specifying the appropriate properties of the fuel and oxidant used in the combustion system and the boundary conditions, such as the flow rate of both the air and the fuel. Then the governing partial differential equations for the reacting gas phase flow may be solved according to the given boundary conditions. The particle specific submodels are used to calculate the particle trajectories, heating up, drying, volatile release and char reactions. These calculations generate and provide updates to the source terms, as well as other relevant parameters and physical properties that are required in the governing partial differential equations for the gas flows. The convergence of the iteration is checked; if the residue of the solution is large than a prescribed tolerance then the calculation should continue with the updated source terms and physical properties until the convergence criteria is

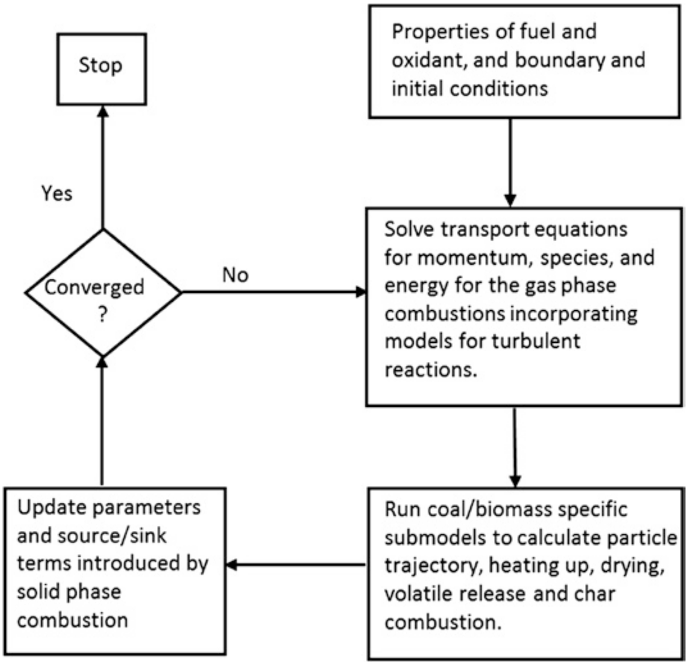

Stop
Properties of fuel and oxidant, and boundary and initial conditions
Yes
Converged ?
No
Solve transport equations for momentum, species, and energy for the gas phase combustions incorporating models for turbulent reactions.
Update parameters and source/sink terms introduced by solid phase combustion
Run coal/biomass specific submodels to calculate particle trajectory, heating up, drying, volatile release and char combustion.

Fig. 6.1 Eularian-Lagrangian approach for modelling co-firing of biomass and coal

satisfied. Most general purpose CFD software packages have these numerical facilities built in. However, those sub-models that are unique to the physical and chemical processes of the solid fuel combustion, in particular for the biomass fuels which are usually quite different from that of coal, have to be specially developed.

6.1.1 Reynolds-Averaged Navier-Stokes Equations

The Reynolds-Averaged Navier-Stokes equations are commonly employed for turbulent reacting flows. Steady state Reynolds-Averaged Navier-Stokes equations and the continuity equation may be written in a Cartesian co-ordinate system as follows:

$$\frac{\partial \rho u^i u^j}{\partial x^j} = -\frac{\partial p}{\partial x^i} + \frac{\partial}{\partial x^j}\left[\mu\left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i}\right)\right] + \frac{\partial \tau^{ij}}{\partial x^j} + \rho g^i + F^i \tag{6.1}$$

$$\frac{\partial \rho u^i}{\partial x^i} = S_m \tag{6.2}$$

where u^i, p, ρ and μ are the mean fluid velocity components, pressure, density and molecular viscosity of the fluid flow, respectively, g^i is the gravitational acceleration and F^i is the source term for the external force, such as the force arisen from the interaction with the dispersed biomass (or coal) particles in the flow. Further,

$$\tau^{ij} = -\rho \overline{u'^i u'^j} \tag{6.3}$$

is the Reynolds stress tensor. This results from the Reynolds average of the Navier-Stokes equations and it represents the effects of the turbulence in the fluid flow, and the overbar denotes a Reynolds average and the dash represents the fluctuating part of the velocity of the fluid flow. This is where a turbulence model comes into the governing fluid flow equations that will be discussed later, which links the Reynolds stress tensor τ^{ij} to the global mean fluid velocity u^i.

In addition to the Navier-Stokes equations, which prescribe the motion of the fluid flow, the energy equation is used to govern the heat transfer within the gas phase and between the gas and the solid phases. The energy equation can usually be written in the following form:

$$\frac{\partial u^i(\rho e + p)}{\partial x^i} = \frac{\partial}{\partial x^i}\left[k_{eff}\frac{\partial T}{\partial x^i} + D_s + \Phi\right] + S_e \tag{6.4}$$

where e, T and k_{eff} are the internal energy, temperature and the effective heat conductivity of the fluid flow, respectively; D_{s} represents the energy transfer due to species diffusions and Φ is a diffusion term; and S_{e} is the energy source term such as heat from a chemical reaction. In coal/biomass combustion simulations, this should also include the heat transfer between the gas and solid particles that are responsible for the heating and cooling of coal or biomass particles.

In a chemical reacting system, the changes in the concentrations of each of the species in the system should follow the basic conservation law and this may expressed in the form of transport equations as follows:

$$\frac{\partial\left(\rho u^{i} Y^{k}\right)}{\partial x^{i}}=-\frac{\partial J^{k}}{\partial x^{i}}+S_{k}, \quad k=1,2,\ldots,n-1 \tag{6.5}$$

where Y^k, J^k and S_k denote the mass fraction, the diffusion flux and the production and destruction of the species k, respectively, during the combustion processes, and n denotes the total number of chemical species involved in the combustion system and this is usually dependent on the knowledge of the composition of the volatiles and the reaction mechanism employed in the numerical simulation. For coal/biomass combustion, S_k should include the source/sink terms resulting from the drying, devolatilisation and char combustion of the coal and biomass.

Equations 6.1–6.5 form the basic set of governing equations for the gaseous phase combustion modelling of the coal and biomass combustion. Additional char combustion models are required providing source term for heat and species mass transfer. Further, appropriate turbulence models have to be used to calculate the Reynolds stress tensor.

It should be noted that there are three fundamental numerical techniques that may be employed to simulate turbulent reacting flows with various degrees of detail along with different computational costs. They are the Direct Numerical Simulation (DNS) technique, the Large Eddy Simulation (LES) technique and the Reynolds-Averaged Navier Stokes (RANS) technique, each of which employs different forms of the fundamental governing partial differential equations.

The DNS technique employs the full Navier-Stokes equations without using any models for the turbulence. This technique requires the computational cells to be small enough to resolve the full spectrum of the turbulent eddy that exist in the fluid flow. This usually results in the use of such a large number of computational cells that makes it not practical for most engineering modelling applications. The LES directly solves for the large scale turbulence that is resolved by the computational grid employed and the remaining sub-grid turbulent eddies are modeled using the so-called subgrid turbulence models. The idea of this is that small scale eddies are mainly responsible for the turbulence energy dissipation and they can be modelled relatively independent to the boundary conditions. Therefore, the size of the computational grid employed in the LES can be much larger than that used in DNS. This can substantially reduce the number of grids required in a CFD model.

The RANS employs the Reynolds-Averaged Navier-Stokes equations given in this section where all the spectrum of the turbulent eddies in the system, from large to small scales, are modelled with appropriate turbulence models. For engineering applications, a number of different turbulence models are now available, each involving different levels of complexity but inevitably all have their limitations in use. With the one equation mixing-length turbulence model being the simplest and the Reynolds Stress Model (RSM) the most complex, the k-ε turbulence models are the most commonly used in various engineering applications, including combustion simulations.

The k-ε model is based on the Boussinesq eddy-viscosity hypothesis which relates the Reynolds stress tensor to the mean fluid velocity through the following equations:

$$\tau^{ij} = -\frac{2}{3}\rho k \delta^i_j + \mu_t\left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i}\right) \tag{6.6}$$

$$\mu_t = c_\mu \rho \frac{k^2}{\varepsilon} \tag{6.7}$$

where μ_t is known as the turbulence viscosity and c_μ is an empirically derived constant and usually takes the value of 0.09. The turbulent kinetic energy k and the dissipation rate ε in the k-ε model are further calculated by two more model transport equations.

As we can see from Eqs. 6.6 and 6.7, the turbulence viscosity μ_t in the k-ε model is a scalar which assumes an isotropy in the turbulence. It is because of this assumption that makes the k-ε model frequently over predict the turbulence viscosity in the situations where non-isotropic turbulence prevails. In pf combustion applications, this occurs where there is a strong swirling flow, such as in the burner near-field and in T-fired furnaces. It should be noted that due to the apparent failings of the standard k-ε model in terms of its inability to account for strong rotational strain or shear, various nonlinear modifications have been developed. Nevertheless, the standard k-ε model is still very widely used in various combustion models and this is largely because of the relative robustness in computations.

For strong swirl flows, a more elaborate RNG k-ε model may be preferred which is also easy to implement and the convergence is robust. The RNG k-ε model is very similar in its formulations to the standard k-ε model. However, an extra term is introduced in the transport equation for the dissipation rate to account for the effect of the anisotropic large-scale eddies giving substantial improvement in the predictions of swirling flows, and flows with a large degree of strain and/or a large boundary curvature.

The Reynolds-Stress Models (RSMs) have emerged as strong candidates for use in industrial turbulent flow calculations. Since the RSMs are second-order closure models which model the different evolutions of the components of the Reynolds stress, $\tau^{i,j}$, separately with different transport equations. Therefore, they are potentially superior to the simpler eddy-viscosity models, such as the k-ε models. However, it is worth mentioning that various Reynolds Stress Models, including those of the simplified Algebraic Stress Models comprise a group of complicated formulations that require a potentially excessive amount of computational effort for the simulation of three-dimensional fluid flows. In addition, it is reported that not all the fluid flow simulations can benefit from the RSMs to justify the high computational costs. This is why even though more sophisticated models have been proposed, the k-ε model with its various modifications is still the most popular turbulence model in use.

6.1.2 Turbulence-Chemistry Interactions

In laminar combustion flows, chemical reactions are usually governed by the Arrhenius equation that can be expressed in general form as:

$$k = AT^{\alpha}\mathrm{e}^{-E/RT} \tag{6.8}$$

where k is the rate constant, α is the non-dimensional temperature exponent, A and E are the pre-exponential factor and the activation energy of the reaction, respectively, and R is the universal gas constant. Once the reaction path for the combustion has been specified then the species production/reduction, as well as heat generations, can be calculated according to the local concentrations of the reactants and the reaction rate with Eq. 6.8. A number of kinetic compilations are available such as Chemkin (Reaction Dynamics 2014) and the CRECK (2014) data.

Pulverised solid fuel combustion is usually in a highly turbulent environment and turbulent gaseous species mixing may play a significant, if not a dominant, role in turbulent combustions of coal and biomass. Chemical reactions in non-premixed combustion, such as the volatile combustion, occur only when the fuel and oxidant come into contact molecularly. Therefore, the relative importance of turbulence on the rate of combustion is determined by the speed at which chemical species come into molecular contact, i.e. the speed of mixing, and the speed at which chemical reaction takes place in the combustion. Volatile combustion is fast and the time scale of the chemical reaction is much smaller than that of the turbulent mixing. Therefore the reaction is mainly mixing controlled. In such cases, the complex chemical kinetic rates can usually be neglected and the fast reaction assumptions, such as ‘equilibrium’, ‘mixing is burnt’ or one or two step global reaction may be employed. The two most frequently used fast reaction modeling approaches are the eddy-breakup model based, such as the eddy-dissipation model, and the other is the mixture fraction model based.

The eddy-dissipation model is a type of eddy-breakup model which calculates the turbulent chemical reaction rate in association with the eddy dissipation/mixing time scale, k/ε. In implementing this model, three different reaction rates may be calculated for each species, namely, the Arrhenius reaction rate, the rate due to the dissipation of turbulent reactant eddies and the rate due to the dissipation of turbulent production eddies. The net rate of production of the species due to reaction is given by the smallest of the three. The eddy-dissipation rate is generally smaller than the Arrhenius rate in mixing-controlled combustion and thus determines the overall reaction rates. It is noted in some gas combustion applications that the Eddy-Dissipation model over-predicts the flame temperatures and it should also note that this model is not appropriate to be used for multi-step reactions since a single reaction rate that is based on the turbulence dissipations is used for all steps.

When multi-step reactions are considered, the eddy-dissipation concept (EDC) model may be employed. EDC is an extension to the eddy-dissipation model that includes the detailed chemical mechanisms in turbulent flows. This model assumes that the reactions proceed according to the Arrhenius rates over the time scale which is defined as a function of the turbulence viscosity and dissipation rate. The Arrhenius rates may be calculated from the detailed chemical mechanisms employed for the turbulent reacting flows. However, it should note that reaction equations have to be numerically integrated time and again when the EDC is employed and it is computationally costly particularly when a large number of reactions are employed for a complex reaction flow.

The mixture fraction model approach has been widely used in coal combustion modelling applications and it is considered to be accurate over the finite rate eddy dissipation models since it can account for multi-species and multi-step reactions. Instead of solving explicitly the conservative equation for the species mass fractions, in the mixture fraction approach the mass fraction of each species, as well as all other thermo-chemical scalars, such as density and temperature, are uniquely related to the mixture fraction and enthalpy through a prescribed probability density function (PDF) of the mixture fraction, such as the delta and beta functions. This greatly reduces the number of conservative equations required to represent a combustion system and thus this saves the computational time.

In the mixture fraction model, when fast chemistry is assumed then an instantaneous reaction occurs as soon as the fuel and oxidant are simultaneously present at the same point. The mixture fraction f for the reaction can be defined by

$$f = \frac{\chi - \chi_O}{\chi_F - \chi_O} \tag{6.9}$$

$$\chi = m_F - \frac{m_O}{r} \tag{6.10}$$

where m is the mass fraction and the subscripts F and O refer to fuel and oxidant, respectively, r is the stoichiometric ratio of the oxidant and fuel by mass. The mixture fraction reflects the degree of mixing of fuel and oxidant in the flow. It can be proved that the mixture fraction f is equivalent to the mass fraction of the fuel in the system and thus it is a conserved quantity and the mean of the mixture fraction, $\bar{f}$, satisfies a conservative transport equation of the form:

$$\frac{\partial}{\partial x^i}\left(\rho u^i \bar{f}\right) = \frac{\partial}{\partial x^i}\left((\frac{\mu_t}{\sigma_t})\frac{\partial \bar{f}}{\partial x^i}\right) + S_f \tag{6.11}$$

where S_f is the source due to the transfer of mass into the gas phase from the combusting solid particles. In addition to the mean values of the mixing, in order to account for the instantaneous values due to the turbulence fluctuation, transport equation for the variance of the mixture fraction is usually solved. Further, chemical reactions are calculated using the appropriate fast reaction models and three key methods exist, namely, mixed-is-burned (or flame-sheet approximation), equilibrium chemistry, and the non-equilibrium chemistry (flamelet). The mixed-is-burned approximation is the simplest reaction scheme which assumes that the chemistry is infinitely fast and the fuel and oxidant do not coexist in space. Therefore, the species mass fractions can be determined directly from the instantaneous mixture fraction through reaction stoichiometry. However, this implies a complete single-step reaction to the final products and often results in a serious over-prediction of the peak flame temperature, especially in an oxygen rich environment. The equilibrium approach assumes that the reaction is fast enough for the local chemical equilibrium to always exist and thus the instantaneous species mass fractions can be calculated based on the minimization of the Gibbs free energy. Equilibrium calculations break down in situations where nonequilibrium prevails, such as in the rich side of flames. The flamelet model on the other hand calculates the instantaneous species mass fractions from the flamelets that have the same structure as laminar flames. The property of the laminar flames may be obtained by either experiments or calculations where a more realistic chemical kinetics effect can be incorporated. However, it should be noted that all the three approaches mentioned here are under the fast reaction assumption. For slow reactions with large reaction time scales, then finite rate chemistry models should be investigated.

When the mixture fraction approaches is employed in the modelling of co-combustion of two dissimilar fuels at least three streams of volatiles combustion need to be tracked separately. This makes the mixture fraction formulations much more complex and computational costly.

6.2 Modelling Pulverised Biomass Particle Combustion

Computer models for the heterogeneous combustion of coal have been relatively well developed because of the commercial needs of the power generation industry. However, models for biomass combustion have not been fully established and need further investigation. In general it is believed that in many cases the major processes of biomass combustion are similar to that of coal combustion. Therefore, modelling approaches that have been specially developed for coal combustion may be extended to the biomass combustion modelling incorporating biomass specific combustion rate constants in the CFD models.

Further, the use of biomass as a fuel presents a problem in that it is difficult to mill into small particles such as coal although treated biomass through torrefaction will improve its milling property. Consequently, pulverised biomass fuel usually contains particles with a larger size and aspect ratio than that of coal. This produces significant complexity in the CFD modelling of the particle aerodynamics and heat and mass transfer that need to be considered.

6.2.1 Particle Motion

In a typical pulverised fuel combustion system, the volumetric flow rate of the solid fuel is usually so small compared with that of the air. Therefore, the fuel particles in the flow stream are usually so far apart that the particles have little chance of interaction. In this situation the particle flow can be treated as dilute in the CFD model and a group of streams of particles over a range of sizes that represent the whole range of particle size distributions are tracked throughout the furnace and the different stages of the particle combustions are then modelled. In the commonly used framework of the Eulerian-Lagrangian modelling approach, the movement of the biomass particles are numerically tracked in the Lagrangian frame of reference and it is governed by the particle momentum equation obtained directly from Newton's second law as follows:

$$\frac{du_p^i}{dt} = F^i \tag{6.12}$$

The left hand side of Eq. 6.12 is the acceleration of the particle and on the right hand side are the forces that are exerted on the particle of unity mass. The forces which commonly act on a particle which is moving within the fluid flow are those which are produced by drag, gravity and, to a lesser extent, the gradients in the fluid velocity, pressure and temperature. For small particles that are suspended in a turbulent flow, additional forces, which are related to the energy which is consumed by putting the medium itself into motion, may be needed to be taken into consideration. There is still a considerable debate on the best way to calculate all these additional forces when modelling a particle that is suspended in a turbulent fluid flow.

In most modelling applications of pf coal combustions, the drag is often the only force that is considered and this is primarily because coal particles are usually small and have a high surface-volume ratio making the drag to be the dominant force over all other forces. The gravity force is also considered in many CFD calculations since it is the main reason for the production of the bottom ash. Since coal particles are not only small and but they tend to melt and become spherical during pyrolysis, therefore coal particles are typically treated as spherical particles in CFD models and thus the drag that acts on the particle by the gas phase can be expressed as follows:

$$F_D^i = C_D \frac{18\mu}{\rho_p d_p^2}\left(u^i - u_p^i\right) \tag{6.13}$$

where ρ_p, d_p and u_p are the density, diameter and the velocity of the particle, respectively. The drag coefficient, C_D, is often experimentally based and expressed as a function of the particle Reynolds number.

Modelling of the motion of biomass particles is much more problematic than that of coal particles. The size of the biomass particle used in the pf furnace is sometimes 10 times larger (in dimensions) than the coal particles and have a large aspect ratio, typically of the order of 10, and with a range of particle shapes such as cheap, disks, cylinders and even needles and fibres. These large biomass particles are prone to the effect of gravity and easily come down to the bottom ash in the furnace, particularly those particles that contain elements, such as the nodes and knots in wood, that are difficult-to-burn. Therefore, the effect of gravity in biomass combustion needs to be considered in the numerical simulations as it may have a significant effect on the model predicted particle trajectories in the furnace, although the effect may not be significant in a pf coal fired combustor with fine coal particles. Further, unlike coal particle that often softens and forms spherical particles during initial devolatilisation, the biomass particles tend to retain their initial form that is irregular in shape. Therefore, it will be inaccurate to take biomass particles as spherical particles as we do for the coal particles in the CFD model, since the shape of the particle has a strong influence on the path of the particle motion in the combustion chamber. There are different ways of dealing with the effect of the particle shape on the particle tracking and in principle this is achieved by considering the aerodynamic effects of the irregularity of the particle with more or less reference to a spherical particle. One way of dealing with the irregularity in the particle shape is to employ the so-called aerodynamic diameter of the particle, which is defined as the diameter of an equivalent sphere which has a unit physical density and the same settling velocity as that of the particle in question. More commonly used ways of modelling the motion of irregular particles is the introduction of a particle shape factor, or sphericity, which is defined as the ratio of the surface area of an equivalent spherical particle, s, and the real particle surface area, S, for example, as follows:

$$\phi = \frac{s}{S} \tag{6.14}$$

Then the drag that acts on a non-spherical particle may be formulated as a function of particle Reynolds number based on experimental data as follows:

$$C_D = \left(1 + a_1 \mathrm{Re}^{a_2}\right) + \frac{\mathrm{Re}}{24} \frac{a_3 \mathrm{Re}}{a_4 + \mathrm{Re}} \tag{6.15}$$

where a_1, a_2, a_3 and a_4 are empirical constants and often expressed as a function of the particle shape factor. The diameter of the sphere of equal volume has been used in the drag and particle Reynolds number calculations. There are numerous other ways of calculating the drag coefficient. Inevitably, there is debate on the accuracy of the formulations in modelling the drag of a vast variety of non-spherical particle shapes and aspect ratios because experiments can only be performed with a limited number of shapes and size of particles. The introduction of the shape factor to some extent represents the effect of the aspect ratio of the particle on the motion of the particle but the details of the particle are not calculated exactly. For disk and chip shaped particles, the particles may be tumbling during their penetration of the highly turbulent gas flow in the furnace, and the drag that is exerted on the particle is significantly influenced by the instantaneous orientation of the particle. However, the instantaneous orientation of a particle is influenced by the initial state of the particle as it enters the computational domain which itself is arbitrary and difficult to determine. More detailed aerodynamics of the flow over irregular shaped object is very complex and is impractical to be modelled in detail. For the purpose of the computational simulation of a group of dispersed fuel particles of vast diversity of shape and size, the practical way of effectively calculating the drag acting on the particles is to use experimental based empirical formulae.

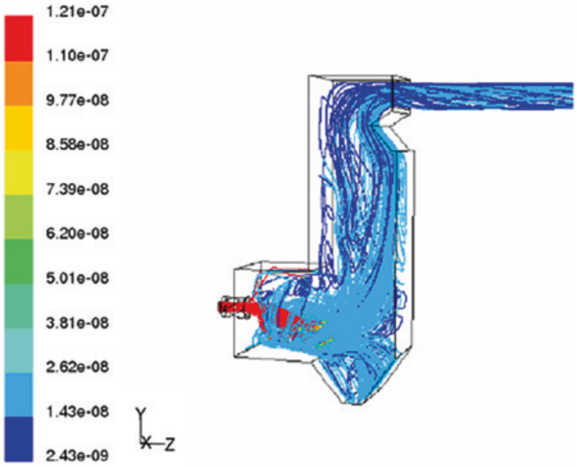


Fig. 6.2 Model predicted biomass particle trajectories in the EON 1 MW combustion test furnace. The initial equivalence particle size is 0.75 mm with a shape factor of 0.1. The scale is *coloured* by particle mass (kg). The EON Test Facility is at Ratcliffe, UK

It is seen in Fig. 6.2 that most of the particles with a shape factor of 0.1 penetrate to the fly ash but some particles do comes down to the bottom of the furnace. However, if the particles were spherical coal particles then all the particles of this size would be expected to end up in the bottom ash. Model predictions show that on decreasing the biomass particle shape factor, i.e. the particle is more non-spherical, then the biomass bottom ash decreases and the fly ash increases.

For particles that are suspended in a fluid flow, in addition to the drag and the gravity, the forces that act on the particles may also include those that are produced by the gradients in fluid velocity, pressure and temperature in the undisturbed fluid flow. Particles traverse in a fluid with a velocity gradient may experience a lift force if the particle is rotating. The pressure difference in the ambient fluid stream also results in a force that acts on the particle and this may become significant when the size of the particle is large. A temperature gradient in the gas flow may also impose a force on the suspended particle, known as the thermophoretic force, in the direction opposite to that of the temperature gradient. This may be significant near to a cooled or heated surface, in particular for submicron particles. However, in most situations, these forces are small for larger particles and can be ignored in most mathematical models. The drag and the gravity forces are the dominant forces that control the motion of the biomass particles in the combustion furnace.

Large particle sizes and aspect ratios also present a number of heat and mass transfer problems for the CFD modelling. For a pulverized coal particle, of say, typically about 50 μm, the particles can be heated up instantaneously. The pyrolysis of such small particles is essentially unaffected by the heat transfer within the particle. Therefore, in the CFD model, the thermal state of a particle can be represented by a single uniform particle temperature. However, for large particles, say 1 mm or larger, a temperature gradient from the surface to the centre of the particle will build up. The thermal and mass transport limitations and the temperature gradients within the particle will have an effect over the life time of the particle as it passes through the furnace. At present, most CFD models ignores the effects of heat and mass transfer within the particle and this is acceptable in coal combustion simulations, as the temperature is fairly uniform inside the small pulverized coal particles and the mass transfer may be so fast so that the carbonization uniformly proceeds throughout the particle. However, the effect of heat transfer within relatively large biomass particles must be accounted for in the CFD simulations.

In order to investigate the instantaneous temperature distribution inside large size and high aspect ratio biomass particles, CFD models may be developed where the heating up process of the particles may be numerically calculated. Figure 6.3 shows the model predicted transient temperatures on the surface and at the centre of the two cylindrical wood particles when they are heated up in a nitrogen gas stream. The two particles have the same diameter, i.e. 9.6 mm, different aspect ratios of 1.0 and 4.0 and moisture content of 6 %. Figure 6.3a, b presents the comparisons of the numerical predictions of the wood particle surface and centreline temperatures with the experimental data. Although the particle surface temperature and centre temperature reach the same value at the end of pyrolysis, larger particles will take a longer time to heat up and have a greater internal temperature gradient. Similar situations exist for biomass fuel particles in pf furnaces. This slow heating up process will significantly affect the pyrolysis, as well as the devolatilisation, of large biomass particles in the combustion, and this may have a significant impact on the flame structure and char burn-out. In addition, for large particles, devolatilisation and char combustion may coexist in different parts of the particle. This is particularly true for irregular shaped particles. However, at present, it is very difficult to model the combustion of such irregular shaped particles in detail in a full scale combustion simulation. Although substantial progress has been made in recent years, accurate sub-models to account for the effect of particle shape on the heat and mass transfer within the particles have yet to be developed and they require a significant amount of effort by both experimentalists and CFD modellers.

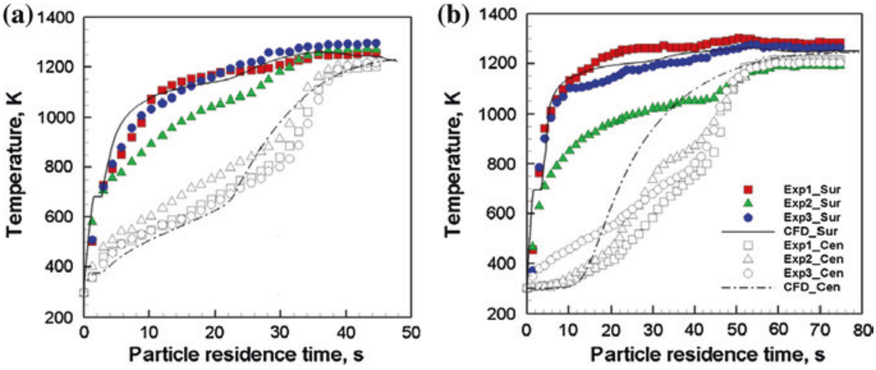


Fig. 6.3 Temporal variations of the surface and centreline temperatures of wood particles of dp = 9.6 mm and moisture content of 6 % (wb) during pyrolysis in nitrogen. **a** Particle aspect ratio 1.0, and **b** particle aspect ratio 4.0

6.2.2 Heat Transfer

Once the particles emerge from the burner, they are heated up by a combination of convective and radiative heat transfer from the furnace walls and hot gases and continuously absorb heat during the processes of volatiles and char combustion. In the CFD model, the heat lost or gained by the particle as it traverses the furnace will be presented as a source or sink of heat in the energy equation for the gas phase.

The instantaneous temperature of a particle travelling in the combustion furnace may be calculated as follows:

$$m_p c_p \frac{dT_p}{dt} = hA_p\left(T - T_p\right) + A_p \varepsilon_p \sigma \left(T_{rad}^4 - T_p^4\right) - Q_{dry} + Q_{reac} \quad (6.16)$$

where m_p is the mass of the particle, c_p is the heat capacity of the particle, A_p is the surface area of the particle, T is the local gas temperature, T_p is the particle temperature, h is the convective heat transfer coefficient, ε_p is the particle emissivity, σ is the Stefan-Boltzmann constant, and T_{rad} is the radiation temperature that is a function of the radiation intensity.

Radiative heat transfer is one of the dominant processes for heating up fuel particles in a large furnace. There are a number of radiation models available for combustion modelling. However, in pf combustion modelling applications, the P-1 model and the Discrete Ordinate model are often employed. The P-1 model is a first-order approximation to the radiation transfer equations by integration where the radiation intensity is represented by a series of spherical harmonics. The Discrete Ordinates radiation model is an approximator for the radiative transfer equation by discretizing the entire solid angle (4π) with a prescribed finite number of solid angles. On increasing the fineness of the angular discretization the accuracy of the model calculations may be improved with an additional cost of computation. There is debate on the use of radiation models in pulverised biomass and coal combustion simultaneously and the temperature field obtained may be dependent on the type of radiation model employed. In general, the P1 model is easy to implement and computationally robust. It is accurate for pulverised coal combustion simulations with radiation scattering, in particular if the optical dimension of the medium is large. The Discrete Ordinates radiation model is more computationally expensive but potentially more accurate.

In addition, as discussed in the previous section, for the usually very small coal particles, there would be a very limited temperature gradient within the particle in a very short period of time and the entire particle can be virtually heated up instantaneously. However, when the size of biomass particles can be up to 20–200 times as large as average pulverized coal particles of say, ~50 μm. Then the thermal-resistance of the particle may produce a noticeable temperature gradient within the particle. This delays the heating up of the biomass particle as a whole and will have a further effect on the subsequent processes of drying, devolatilisation and char combustion. Therefore, a delay in the ignition of the biomass particle can be observed. The stability of the flame will also be influenced by the rate of the heating up of the particles, in addition to the heating values of the fuel. Therefore, for a thermally thick large biomass particle, where there exists a significant temperature gradient within the particle, then additional heat balance models within the particle have to be developed in which both thermal-physical properties and the shape and dimensions of the particle may be considered.

6.2.3 Devolatilisation

The process of devolatilisation was discussed earlier in Sect. 3.3. In biomass CFD models it plays a very important role because of the large quantity of volatiles produced. In most coal models, the process of drying can be incorporated in the devolatilisation model. However, in biomass combustion, the water content is usually larger and in some instances it may dominate the combustion process. Consequently, the drying step is often treated as a separate process as set out earlier in Eq. 3.1.

The rate of volatile release determines the volatile mass transfer from the solid particle to the gas phase and the subsequent volatile gas combustion. As previously described there may be catalytic effects which complicate the process. The input data are the reaction kinetics for the particular biomass using experimental data or information from one of the network codes described earlier. At present there is a considerable amount of data suitable for fixed bed combustion but not much available for higher temperature pf furnaces. Network codes may be used and whilst they may be applicable to commonly used biomass the range covered at present is not large. This is in contrast to the wealth of information available on coal because of long established commercial interests of the coal industry.

The other inputs required are usually the proximate and ultimate analyses and the high temperature volatile yield which is higher than that given by the Proximate Analysis. This value can be obtained from the Network Codes or determined experimentally. Then the rates and yields of all major species, molecular weight distributions and elemental compositions of tar and char from the fuel undergoing devolatilisation can be predicted and used for CFD model inputs. Thermal data such as specific heats as well as densities are also required for the heating-up models.

The devolatilisation process for a particular biomass may be modelled in the CFD model with different levels of complexity. The simplest model is to assume a constant rate of devolatilisation, the single kinetic reaction model, where typically representative values for both the devolatilisation rate and devolatilisation temperature may be used so that the overall process of the volatile release can be modelled. In this situation, the rate of volatile release may be assumed to be first-order dependent on the amount of volatiles remaining in the particle as previously described in Chap. 3. However for accurate modelling of the lower temperature processes such as ignition or the combustion of thermally thick biomass then the use of a three stage devolatilisation model is the best approach.

6.2.4 Char Combustion

The main features of char combustion were considered in Chap. 3. Char combustion occurs principally after the end of the devolatilisation, although in practice a small fraction of char oxidation begins earlier and co-exists with the devolatilistion step. Char combustion is a much slower process and therefore it determines the extent of burn-out of the solid fuel in the furnace; this is experimentally measured as the carbon-in-ash, i.e. the carbon remaining in the ash at the exit of the combustor. In typical large-scale pulverised fuel plants the furnace residence time is of the order of several seconds to allow for complete char burnout. Similar furnaces are used for the combustion of biomass and although the char accounts for a much smaller fraction of biomass fuels, firing large biomass particles in the existing pulverized coal furnace may raise concerns over unburned carbon.

Similar factors apply to combustion in fixed, travelling or fluidised beds. That is, the overlapping devolatilisation and char burnout stages and the concern about unburned carbon remaining in the ash. An extra concern in the combustion of fixed bed combustion is the inhibiting effects of ash which can form a layer on the outside of the char particle. In pf combustion the motion of the particle may remove much of this ash and this is the case in travelling and fluidised bed combustion too. In fixed beds with for example this has to be taken into account (Mehrabian et al. 2014).

The critical step is the calculation of the rate at which solid char particles is oxidised. Coal char combustion can be modelled relatively accurately but this is not yet the case of biomass. The burnout rate is more complicated as it is affected not only by the composition of the biomass fuel but also by the shape and size of the particles and therefore the heating-up process as previously outlined. A further complication is that biomass used in real world reactors generally consists of mixtures of woods and may contain bark, roots and impurities such as soil. The milled biomass is not uniform chemically and in the case of wood it contains ‘knots’ which have a higher lignin content and are thus less reactive. This is also true for ‘nodes’ in Miscanthus and ‘knees’ in straw.

There is a paucity of reactivity data available for biomass char at high temperatures and is often conflicting. The combustible portion of both coal and biomass char particles is basically the solid carbon. The abundant inorganic elements in the biomass char particles tend to remain within the ash. As soon as the fixed carbon on the surface of the char particles is molecularly in contact with the oxidant from the gas phase then the reaction proceeds and produces the gas phase products. At the high temperatures that typically occur in the pf combustion furnace, diffusion is more likely to be the control mechanism of the entire char combustion than the chemistry. For biomass particles, large aspect ratios are usually a typical feature and any shape from plates, chips or round cylinders to needles and fibres may be present. The immediate effect of this is the increased surface area of the particle compared with the equivalent spherical particle and this would enhance the diffusion of the oxidant to the pores within the biomass char particles.

Metal and inorganic elements account for a fairly large percentage of char mass and thus may effect on the combustion rate of biomass chars. There is a considerable uncertainty about the role of catalytic metals in char combustion. Generally it is believed that at high temperature char combustion in pf furnaces, where a very fast chemistry exists, the catalytic effect is not as significant as it is in low temperature combustion. Further, biomass chars contain high levels of oxygen and low levels of hydrogen which tend to prevent graphitic structures from developing in biomass chars.

6.3 Modelling Pulverised Fuel Co-firing in Power Stations

Co-firing coal and biomass in a pf furnace involves the simultaneous combustion of a blend of two very different fuels in terms not only of their different chemical compositions and reactivity during combustion, but also different particle aerodynamics and heat and mass transfer. The combustion behaviours of two dissimilar types of solid fuels have significant nonlinear characteristics. When co-firing coal and biomass in a pf coal furnace, the vast differences in the combustion properties of biomass have a noticeable impact on the combustion of coal, see for example, Kaer et al. (1998) and van Loo and Koppejan (2008).

In CFD simulations, pf solid fuel combustion is usually modelled in the Eulerian-Lagrangian framework where the motion of particles is tracked individually in a Lagrange frame of reference. When two very distinct fuels are fired simultaneously, then two types of volatiles with different compositions are produced and two types of char particles are formed. Therefore, in the co-firing modelling, up to four different fuel streams need to be tracked in order to model the different processes of drying, devolatilisation, volatile combustion and char combustion in the furnace with precision and, in particular, capture the nonlinear interactions of coal and biomass combustion processes. This put significant demand on both the mathematical formulations and computational techniques.

It would be more or less straightforward to model an additional fuel's combustion by using the eddy break up type of models, such as the Eddy-Dissipation turbulence-chemistry interaction model for volatile combustions. In this situation, the additional biomass volatile and char combustions can be modelled by putting additional source terms into the appropriate conservation equations, such as the energy equation, as well as in the mass and chemical species conservative equations. Clearly, the composition of the biomass volatiles, biomass volatile oxidation reaction mechanisms and the heating values have to be prescribed and this, however, also involves significant uncertainty. With the Eddy-Dissipation model, both volatile and char combustion are modelled as global reactions and therefore intermediate reactions and species could not be calculated.

The mixture fraction approach is also used to model the co-firing of different solid fuels, which is believed to give more accurate predictions of the turbulent gas combustions than does the Eddy-Dissipation type of models. However, the mathematical formulations with the multi-mixture fraction approach would become very complex for co-firing two distinctive solid fuels and this would cause problems in the numerical solution techniques.

There have been a number of attempts to model the blends of coal and biomass combustion using the multiple mixture fraction approach, such as Yin et al. (2010), Abbas et al. (1994), Dhanaplan et al. (1997) and Sami et al. (2001). Various simplifying assumptions have to be made to reduce the level of complexity of the computations. In a simple case, for example in the case of two fuels and the oxidant is shared amongst them, then the mixture fractions can be defined by:

$$f_i = m_{F,i} + \frac{m_{P,i}}{1 + r_i}, \quad \mathrm{i} = 1, 2 \tag{6.17}$$

where m is the mass fraction and the subscripts F, P and O refer to the fuel, products and oxidant respectively. The mean of both mixture fractions Fi, plus their variance, satisfy the standard transport equation for a conserved quantity. Then the equations for the mass fractions of fuel may be solved and the oxidant is shared between the two fuels. Then the mass fractions of the oxidant and products may be obtained from:

$$m_{P,i} = (1 + r_i)(f_i - m_{F,i}) \tag{6.18}$$

$$m_O = 1 - m_{F,1} - m_{F,2} - m_{P,1} - m_{P,2} \tag{6.19}$$

Some detailed formulations for two stream mixture fraction calculations may be found in, for example, the commercially available CFD software ANSYS FLUENT manual. It can be expected that the formulations for three-stream mixture fractions, which are required in order to treat two different off-gases separately for a co-firing application, will become extremely complex and the solution of the mixture fraction equations, the setup of the lookup table and the data retrieval will be much more complex and computationally time consuming.

There are a number of commercially available CFD codes that model coal combustion and NO_x formation with reasonable accuracy. However, handling of two different solid fuels is not yet a typical feature of the commercially available CFD software codes and there are very few full-scale CFD simulations of co-firing in the open literature. This, to some extent, reflects the difficulties in modelling the co-firing of different fuels.

Within the framework of the Eulerian-Lagrangian approach, Backreedy et al. (2005) performed a full three-dimensional CFD modeling of co-firing pine wood and bituminous coal in a 1 MW industrial combustion test facility. The general approach taken was to assume that many aspects of the coal and biomass combustion processes are common, and that the key sub-models used, such as those applicable to drying, devolatilisation, volatile and char combustion, are the same as for coal with different model constants being applied to the two fuels and a kinetic-diffusion model for the biomass char particles. The particle shape factor approach has been used to calculate the effect of the non-spherical shape of the biomass particles on the drag that acts on the particles. The eddy dissipation model was employed for the turbulence chemistry interaction and the RNG model for turbulent swirling flow. The coal char combustion model was based on Smith's model (described in Chap. 3) and this was modified to allow for the effects of macerals, variable surface area and annealing on the burnout of the char, described by Backreedy et al. (2005) and references therein. The P1 model for radiation and the thermal/prompt/fuel mechanisms NO_x have been employed. For biomass combustion, the formation of biomass volatiles and char are calculated by using the FG-Biomass network programme in order to estimate the amount and rates of the volatile release. In this particular study, a smaller amount of biomass has been used in the co-firing, 3 % by mass, and the work focused on the effect of the particle shape and size, volatile release rate and the char burnout rate on the unburned carbon in biomass ash. The study showed that, for the pine wood investigated, small particles, less than about 200 μm, burn out completely. However, the burnout of large biomass particles depends on both the size and shape of the particle and burning rates.

Gera et al. (2002) performed a simulation for the co-firing of coal and biomass switchgrass in a utility T-fired 150 MWe boiler and 10 % (by heat) switchgrass and 90 % coal was used. Again, an Eulerian-Lagrangian approach is used. The simulation uses the standard k-ε turbulence model for the turbulent fluid flow and the eddy dissipation model for the turbulence-chemistry interaction. The radiation model employed is the Discrete Ordinate model. For the biomass char combustion, a diffusion controlled rate model was assumed taking into considerations of the effect of large aspect ratios of biomass particles on carbon burnout where temperature gradient inside the biomass particles is also considered. There are some other similar modelling papers on co-firing which employed different CFD codes, such as Abbas et al. (1994), Dhanaplan et al. (1997) and Yin et al. (2010). The simulations were primarily based on relatively well developed coal combustion sub-models with some modifications and/or further developments in order to make them applicable to the unique features of biomass fuels in terms of both chemical reactions and particle aerodynamics.

Since biomass usually has a lower heating value therefore more biomass fuel will be required in order to keep the same thermal input. This increase in the fuel flow rate

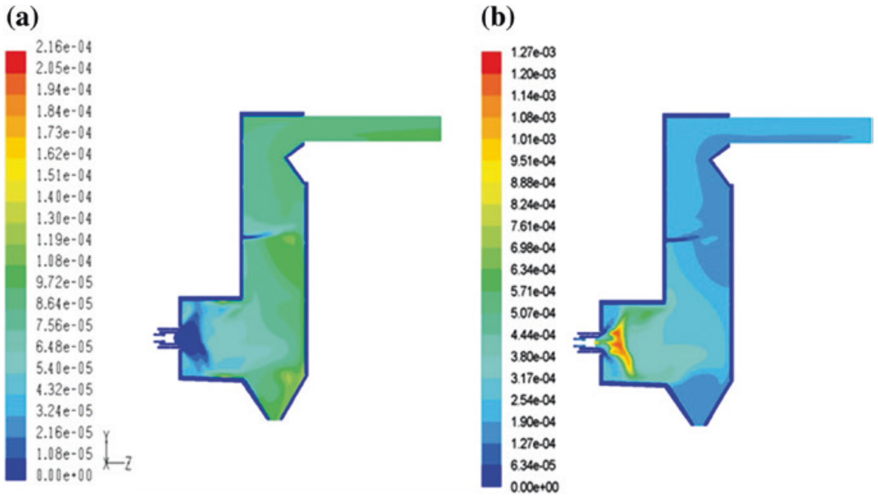
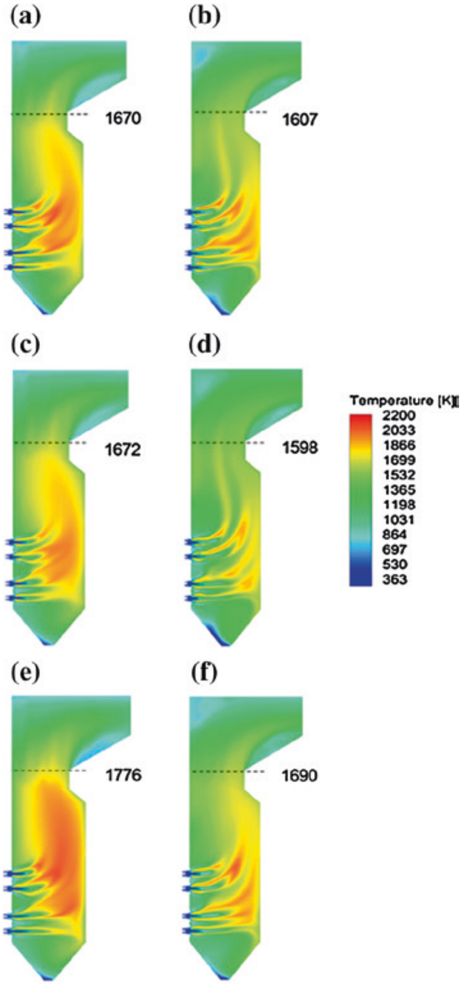


Fig. 6.4 Computed. **a** NO and **b** HCN profiles-same reactor as Fig. 6.2

Fig. 6.5 An example of modelling combustion in a power station boiler using coal or biomass as the fuel, with different levels of oxygen. Temperature distribution **a** air–coal, **b** air–biomass, **c** oxy25 %-coal, **d** oxy25 %-biomass, **e** oxy30 %-coal, and **f** oxy30 %-biomass (Black et al. 2013, with permission)



may cause the flame to move away from the burner mouth, thereby creating a flame stability problem and cause higher emission levels. If pure biomass is used then the whole combustion processes or the combustor itself may need to be changed to suit an efficient combustion of the fuel with, for example, different air splits in the burner.

The modelling of the combustion of small pulverised biomass particles is readily undertaken using CFD methods, although the modelling of the release of the pollutants is much harder. Many studies have been made of pf coal combustion and in a similar way; studies have been made of co-firing using a two-component fuel. Since the amount of biomass is often less than 20 % thermal the main flame properties such as temperature or velocity are largely determined by the coal combustion processes. The key to the correct prediction of NO_x is the correct prediction of the temperature distribution in the furnace especially if staged burners are used.

In large pf-fired, multi-burner furnaces, which use 20 % or more biomass overall, the pulverised biomass is injected via individual biomass burners using 100 % biomass. There have been only a few such studies. Ma et al. (2007) have studied the combustion of pulverised wood and determined NO_x and unburned carbon in ash in a 1 MW Combustion Test Facility. Typical computed profiles for NO_x and the intermediate HCN are shown in Fig. 6.4.

The amount of NO computed on the basis that the fuel-N converts to HCN and then reacts to NO using the ANSYSY FLUENT kinetics is 89 ppm, whereas if the NH_3 mechanism is used it is 266 ppm, the former being closer to the experimental results. In the case of most other fuels it is postulated that the latter is the main route, although it has been observed in industry that the injection of biomass in co-firing does not produce the expected reduction in NO associated with ammonia injection.

An example of modelling combustion in a power station boiler using coal or biomass as the fuel and different levels of oxygen is shown in Fig. 6.5. Temperature distribution (a) air–coal, (b) air–biomass, (c) oxy25-coal, (d) oxy25-biomass, (e) oxy30-coal, and (f) oxy30-biomass.

6.4 Modelling Fixed Bed Combustion

Much of the early work on modelling pollutant formation from grate combustor has been summarized by Saastamoinen et al. (2000). There have been significant advances since then in the chemistry and physics of modelling such combustors and these have been recently described by Mehrabian et al. (2012, 2014). In general modelling presents a number of problems because, whilst the gaseous combustion occurring in the furnace chamber above the surface of the bed is relatively easy to simulate, this is not true of the bed itself. The bed consists of irregular shaped particles where the initial fuel size may be 10–100 mm more, and whilst the term ‘fixed’ is used, in a real system the bed particles are constantly shrinking in size and the bed is moving. This is clear from Fig. 2.2. The fuel is often fed on a batch basis and in addition the bed is not fixed in space and holes can appear through the bed in a random manner. Moving or travelling grate furnace arrangements are simpler in many respects in that input and movement of the fuel particles in the bed can be treated more easily in a statistical manner, although channelling still occurs. Many of the modelling studies undertaken relate to simplified systems and directed to increasing furnace efficiency which can directly reduce pollutant formation, but few modelling studies have been concerned directly with pollution formation. The introduction of wood pellet burners in the last decade has simplified these calculations since the fuel is more uniform and combustion much more consistent. Many researchers have carried out simulation studies of biomass combustion for large particles and pellets as discussed in this chapter.

Some modelling studies have been made of pollutants formed from small village cook stoves. Bhaskar Dixit et al. (2006) and Kausley and Pandit (2010) studied flow and heat transfer in cook stoves but not pollutant formation. Ndiema et al. (1998)

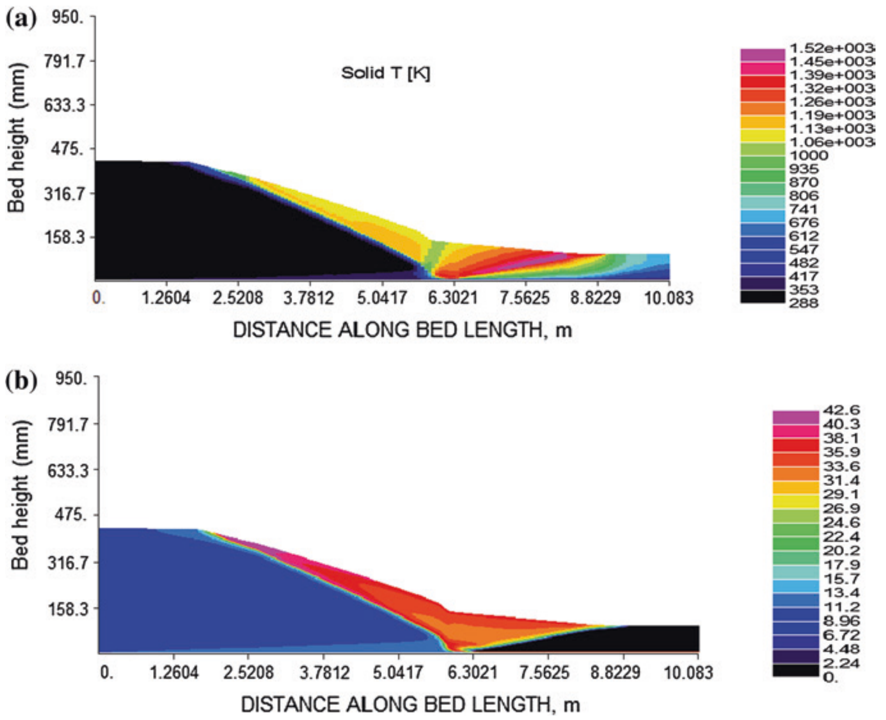


Fig. 6.6 Modelling moving grate combustion showing. **a** Temperature profile inside a grate bed the temperature of the solid bed is in K. **b** Carbon profile inside a grate bed (Yang 2014, Personal Communication, Biomass Power Ltd., UK)

investigated the formation of NO_x, methane and smoke experimentally in a 1-D plug flow model of a cook stove, and the gaseous pollutants followed by Chemkin (2014) modelling. Here the factors determining the methane emission were examined.

A number of studies have been made of larger fixed bed combustors for residential and commercial applications combustion using a variety of fuels (Galgano et al. 2006; Huttunen et al. 2006a, b). The earlier published modelling studies were related to the use of fuels such as wood with an irregular size or briquettes made of sawdust or straw. Later studies were much more general and looked at the influence of the many factors involved such as bed size, level of moisture, particle size etc. Cylindrical pot furnace studies are useful because of the consistency of the combustion process, and this has been used to investigate NO_x formation from several woods and wood pellets. Because of intermittent combustion in practical systems, the complex gas flow, heat transfer and reaction within the bed, many models have been concerned efficiency studies or partial modelling of pollutant formation in the combusting gases above the bed. The introduction of pellet burners in the last decade has not only improved combustion but simplified these calculations since the fuel is more uniform and the feeding process and combustion much more consistent. Recently researchers have carried out simulation studies of biomass combustion for large particles and pellets and calculated NO formation (Klason and Bai 2007).

Modelling the emission of pollutants from larger thermal capacity (about tens of MW) grate units follows the same modelling methods, although the gas flows, especially in the injection of secondary air and in the heat exchanger section, are more complex. CFD modelling in these furnaces has been extensively reviewed by Yin et al. (2008). This review shows how little work has been devoted to modelling pollutant formation in biomass combustion. There are a number of examples related to both fixed bed and travelling grate combustion. Yang et al. (2005) simulated packed-bed combustion of biomass particles with size ranging from 5 to 35 mm. A typical computation for a travelling grate is given in Fig. 6.6.

Whilst most of the studies have been concerned with the major fuels, of wood and straw, some studies have also been made of other biomass materials such as bagasse.

6.5 Modelling Fluidised Bed Combustion

Fluid bed combustion is one of the major methods of utilizing biomass for power generation. A considerable number of plants are installed using a variety of different types of biomass, being particularly suitable for wet agricultural residues. The designs are largely based on those for coal combustion and two types of designs are used, namely bubbling fluidized bed (BFB) and circulating fluidized bed combustors (CFBC), both of which operate with bed temperatures of about 800 °C. The main difference between coal combustion and biomass combustion are the large amount of volatiles produced in the latter case, the greater reactivity, and lower SO_x and NO_x (and N_2O) emissions. Thus the BFB system is suitable for many applications, where neither staged combustion nor in-bed sulphur removal are necessary. It also has the advantage that large particle sizes are possible and less prone to bed agglomeration due to the alkali metals in the ash. Typical sizes are 50–100 MW and, as such, are capable of using major pollution control equipment. Large plant of this type usually has to conform to National Emission Directives and so the level of emission has to be achieved by a combination of the combustion chamber design and the flue gas clean-up plant, which will involve particulate and possibly NO_x units. If the K, Cl, Si contents are high, this can lead to submicron emissions. As with most large-scale combustors the amount of NO_x and the metals can be determined by equilibrium modelling.

6.6 Modelling Pollutant Emissions

6.6.1 Nitrogen Oxides

The modelling of biomass has followed the methods used for coal combustion. In the latter case, considerable attention has been directed to the combustion of pulverised coal, which is the major industrial use of coal, and much less attention directed to fluidised bed combustion and fixed bed combustion. This is the same order of difficulty in modelling. In modelling pollutant formation much more attention has been directed to the gases, NO and CO than to the particulates. Here the outcomes of some major examples of modelling of pollutant formation will be considered.

Similar to coals biomass contains nitrogen although may in a different level and form. When biomass is burnt it produce nitrogen oxides but because furnace temperatures are kept fairly low to prevent slagging the production of thermal-NO_x is low. The fuel-nitrogen is mainly released into the volatiles. Volatile combustion is usually considered as a mixing controlled fast reaction and thus the detailed reaction mechanisms can usually be ignored and global one step or two step kinetics are usually employed. However, in the situation where slow reactions and intermediate species dominant, such as NO_x and SO_x reactions, then finite reaction schemes have to be considered.

There are many studies on NO_x formations for coal combustions, but most are focused on thermal and prompt formation routes which are the key pathways of NO_x formation in high temperature combustions, such as coal and nature gas flame. For biomass combustion occurring at a relative low temperature, the fuel bound nitrogen will be the focus of the investigation of the NO_x formation. The fuel bound nitrogen is typically released in the form of either HCN or NH_3 during combustion before being transformed into N_2 or NO. The exact fraction of each intermediate species formed remains the subject of ongoing research, and this will affect the model prediction of the overall NO_x formation. However, it is generally accepted that ammonia is the principal product of fuel-nitrogen conversion in biomass fuel stocks which may be orders of magnitude higher than those of other fuel-nitrogen species, for example see Zhou et al. (2005). At the moment, quantitative modelling of NO_x formation in biomass combustion is still at an early stage of research.

6.6.2 SO_X Emissions

The sulphur content in the biomass is small; therefore combustion of biomass fuel itself has not become a big issue in SO_x formation except in relation to fine particulate formation where even a small amount of S may be significant. The formation of acid rain is not really an issue with biomass firing although the global effects on the climate are significant. The major concern is during co-firing with coal in large electricity generation units where SO_x up to the permitted limits may be emitted. However co-firing biomass with coal in normally 100 % coal fired plants permits a reduction in the overall SO_x emissions which may result in desulphurisation plant running at a reduced load or not being needed.

6.6.3 Modelling Aerosol Pollutants

Aerosols generated from biomass combustion can be a result of an incomplete combustion such as soot, polyaromatic hydrocarbons (PAH) as well as fragments of ash (Eriksson et al. 2014). However, majority of the aerosols are produced as a result of alkaline metal and chlorine presents in the biomass which lead to the formation of sticky and corrosive components and submicron particulates, such as KCl and K_2SO_4. As discussed before, the form in which the metal species are released from combustion of biomass depends on the relative contents of the potassium and chloride in the biomass. Once released as a part of the volatile, and the oxidation gaseous of char to a less extent, the potassium and chlorine undergo a series of chemical and physical transformation steps to form more stable KCl and K_2SO_4 compounds in gaseous phase and then through nucleation and condensation to form aerosols. The detailed kinetics of the sulphation of alkali spices involves hundreds of intermediate reactions, which are too complicated for use in computational fluid dynamics calculations (Garba et al. 2012). Reduced reaction mechanisms are usually employed and the major reactions include (Glarborg and Marshall 2005):

$$\mathrm{KCl} + \mathrm{H_2O} = \mathrm{KOH} + \mathrm{HCl} \tag{R 6.1}$$

$$\mathrm{KCl} + \mathrm{SO_3} = \mathrm{KSO_3Cl} \tag{R 6.2}$$

$$\mathrm{KSO_3Cl} + \mathrm{H_2O} \rightarrow \mathrm{KHSO_4} + \mathrm{HCl} \tag{R 6.3}$$

$$\mathrm{KOH} + \mathrm{SO_3} \rightarrow \mathrm{KHSO_4} \tag{R 6.4}$$

$$\mathrm{KHSO_4} + \mathrm{KCl} \rightarrow \mathrm{K_2SO_4} + \mathrm{HCl} \tag{R 6.5}$$

The concentration and transportation of the aerosols from KCl and K_2SO_4, as well as other particulates e.g. soot particles, can be modelled using the standard transport equations in the form such as (Jöller et al. 2007):

$$\frac{\partial \rho \phi}{\partial t} + \frac{\partial \left(\rho u^i \phi \right)}{\partial x^i} = \frac{\partial}{\partial x^i} \left(\Gamma \frac{\partial \phi}{\partial x^i} \right) + S_\phi \tag{6.20}$$

where φ is the mass fraction of the aerosol, Γ is the diffusivity and S_ϕ is the production of the aerosol.

The aerosol formation and growth in a combustion system may through both homogenous and heterogeneous nucleation and condensation. Based on classic kinetic theory, homogenous nucleation rate may be given in the form (Hagen and Kassner 1984)

$$J = C^* F A^* a Z \tag{6.21}$$

where C^* is the concentration and A^* is the surface area of critical sized nucleation embryos, F is the flux of molecules to the cluster surface, a is the sticking coefficient, and Z is the Zeldovich factor which accounts for non-equilibrium effects in the embryo concentration. The condensation rate of the species to a particle is a function of vapour pressure, p and saturate pressure $p_{sat,p}$ at the particle surface temperature, typically expressed in the form:

$$m = c \frac{(\dot{p} - p_{sat,p})}{RT} \tag{6.22}$$

where c is mass transfer coefficient, R is the gas constant and T is the gas temperature.

Coagulation of particles due to particle collisions among each other may also be considered. The coagulation process would not influence the total concentration of the particles but does have an impact on the particle size distributions and particle composition. Thus nucleation, coagulation and condensation of alkali and chlorine species are responsible for the formation of majority of the submicron aerosol emissions from biomass combustion. The concentrations of KCl and K_2SO_4 in the flue gas of a power generation boiler also have significant impact on the fouling potentials on the heat exchangers.

References

Abbas T, Costen P, Kandamby NH, Lockwood FC, Ou JJ (1994) The influence of burner injection mode on pulverized coal and biomass cofired flames. Combust Flame 99:617–625

Andersson B, Andersson R, Hakansson LH, Mortensen M, Sudiyo R, van Wachem B (2012) Computational fluid dynamics for engineers. Cambridge University Press, Cambridge

ANSYS FLUENT (2014) ANSYS Inc., USA

Backreedy RI, Fletcher L, Jones JM, Ma L, Pourkashanian M, Williams A (2005) Co-firing pulverised coal and biomass: a modelling approach. Proc Combust Inst 30:2955–2964

Bhaskar Dixit CS, Paul PJ, Mukunda HS (2006) Part I: experimental studies on a pulverised fuel stove. Biomass Bioenergy 30:673–683

Black S, Szuhánszki J, Pranzitelli A, Ma L, Stanger PJ, Ingham DB, Pourkashanian M (2013) Effects of firing coal and biomass under oxy-fuel conditions in a power plant boiler using CFD modelling. Fuel 113:780–786

Chemkin (2014) Reaction design. www.Reactiondesign.com

Chung TJ (2002) Computational fluid dynamics. Cambridge University Press, Cambridge

CRECK (2014) http://creckmodeling.chem.polimi.it

Dhanaplan S, Annamalai K, Daripa P (1997) Turbulent combustion modelling coal: biosolid blends in a swirl burner. Energy Week vol IV, ETCE, ASME, Jan 1997, pp 415–423

Eriksson AC, Nordin EZ, Nyström R, Pettersson E, Swietlicki E, Bergvall C, Westerholm R, Boman C, Pagels JH (2014) Particulate PAH emissions from residential biomass combustion: time-resolved analysis with aerosol mass spectrometry. Environ Sci Technol 48:7143–7150

Galgano A, Di Blasi C, Horvat A, Sinai Y (2006) Experimental validation of a coupled solid- and gas-phase model for combustion and gasification of wood logs. Energy Fuels 20:2223–2232

Garba MU, Ingham DB, Ma L, Porter RTJ, Pourkashanian M, Williams A, Tan HZ (2012) Prediction of potassium chloride sulfation and its effect on deposition in biomass-fired boilers. Energy Fuels 26:6501–6508

Gera D, Mathur MP, Freeman MC, Robinson A (2002) Effect of large aspect ratio of biomass particles on carbon burnout in a utility boiler. Energy Fuels 16:1523–1532

Glarborg P, Marshall P (2005) Mechanism and modeling of the formation of gaseous alkali sulfates. Combust Flame 141:22–39

Hagen DE, Kassner JL Jr (1984) Homogeneous nucleation rate for water. J Chem Phys 81:1416–1418

Huttunen M, Saastamoinen J, Kilpinen P, Kjaldman L, Oravainen H, Bostrom S (2006a) Emission formation during wood log combustion in fireplaces—part I: volatile combustion stage. Prog Comput Fluid Dyn 6:200–208

Huttunen M, Saastamoinen J, Kilpinen P, Kjaldman L, Oravainen H, Bostrom S (2006b) Emission formation during wood log combustion in fireplaces—part II: char combustion stage. Prog Comput Fluid Dyn 6:209–216

Jöller M, Brunner T, Obernberger I (2007) Modeling of aerosol formation during biomass combustion for various furnace and boiler types. Fuel Process Technol 88:1136–1147

Kaer SK, Rosendahl L, Overgaard P (1998) Numerical analysis of co-firing coal and straw. In: Proceedings of the 4th European CFD conference, Athens, Greece, 7–11 Sept 1998, 1194–1199

Kausley SB, Pandit AB (2010) Modelling of solid fuel stoves. Fuel 89:782–791

Klason T, Bai XS (2007) Computational study of the combustion process and NO formation in a small-scale wood pellet furnace. Fuel 86:1465–1474

Ma L, Jones JM, Pourkashanian M, Williams A (2007) Modelling the combustion of pulverized biomass in an industrial combustion test furnace. Fuel 86:1959–1965

Mehrabian R, Zahirovic S, Scharler R, Obernberger I, Kleditzsch S, Wirtz S, Scherer V, Lu H, Baxter LL (2012) A CFD model for thermal conversion of thermally thick biomass particles. Fuel Process Technol 95:96–108

Mehrabian R, Shiehnejadhesar A, Scharler R, Obernberger I (2014) Multi-physics modelling of packed bed biomass combustion. Fuel 122:164–178

Ndiema CKW, Mpendazoe FM, Williams A (1998) Emission of pollutants from a biomass stove. Energy Convers Manag 39:1357–1367

Saastamoinen JJ, Taipale R, Horttanainen M, Sarkomaa P (2000) Propagation of the ignition front in beds of wood particles. Combust Flame 123:214–226

Sami M, Annamalai K, Wooldridge M (2001) Co-firing of coal and biomass fuel blends. Prog Energy Combust Sci 27:171–214

van Loo S, Koppejan J (eds) (2008) The handbook of biomass combustion and co-firing, Earthscan, Washington, DC

Wendt JF (ed) (2009) Computational fluid dynamics: an introduction, 3rd edn. Springer, Berlin

Williams A, Pourkashanian M, Jones JM (2001) Combustion of pulverised coal and biomass. Prog Energy Combust Sci 27:587–610

Yang YB, Ryu C, Khor A, Yates NE, Sharifi VN, Swithenbank J (2005) Effect of fuel properties on biomass combustion Part II. Modelling approach-identification of the controlling factors. Fuel 84:2116–2130

Yin C, Rosendahl LA, Kaer SK (2008) Grate-firing of biomass for heat and power production. Prog Energy Combust Sci 34:725–754

Yin C, Kaer SK, Rosendahl L, Hvid SL (2010) Co-firing straw with coal in a swirl-stabilized dual-feed burner: modelling and experimental validation. Bioresour Technol 101:4169–4178

Zhou H, Jensen AD, Glarborg P, Jensen PA, Kavaliauskas A (2005) Numerical modeling of straw combustion in a fixed bed. Fuel 84:389–403